

# Model Validation Methods for Phase Diagram Determination

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## Abstract

The accurate determination of phase diagrams through modeling is of paramount importance to the nuclear fuels industry as well as to countless other industries operating in multi-component phase fields. However the amount and quality of experimental data is often limited. Likewise, the number and quality of available phase field models are often limited and conflicting in their predictions. This work proposes a method of integrating sparse uncertain experimental data sets with models of various levels of thermodynamic sophistication such that a quantitative determination can be made as to which model is most reliable given the data available. This approach uses a heuristic optimization technique, which is free of assumptions about the uncertainty distributions around data points. The heuristic optimization then provides a distribution-free assessment of the prediction of each model. The predictive spread of each model is compared to the known data (including expert judgments) of the phase fields using standard goodness of fit and generalized information theory comparison techniques. This presentation will show the application of this approach on the calculation of the UO<sub>2</sub>-PuO<sub>2</sub> phase diagram using four different phase equilibrium models for the liquidus and solidus curves.

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